CEWES MSRC/PET TR/98-40

Contract Year Three Programming Environment and Training (PET) Core Support and Focused Efforts for CEWES Major Shared Resource Center (MSRC)

April 1998

DoD HPC Modernization Program
Programming Environment and Training
CEWES MSRC

07h00598

Work funded by the DoD High Performance Computing Modernization Program CEWES Major Shared Resource Center through

Programming Environment and Training (PET)

Supported by Contract Number: DAHC 94-96-C0002
Nichols Research Corporation

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April 1998

Prepared For:
CEWES MSRC
U.S. Army Corps of Engineers
Waterways Experiment Station (CEWES)
Vicksburg, MS

BACKGROUND

As a result of the Annual Review for the U.S. Army Corps of Engineers Waterways Experiment Station (CEWES) Major Shared Resource Center (MSRC) Programming Environment and Training (PET) program that occurred on 24-26 February 1997, a follow-on series of Core Support and Focused Efforts have been funded. These cover the primary Computational Technology Areas (CTAs) supported by the center and other specialty areas, including Scientific Visualization (SV), Scalable Parallel Programming (SPP) Tools, support for Historically Black Colleges and Universities (HBCUs) and Minority Institutions (MIs), Training, and Collaboration/Communication (C/C). The primary CTAs supported at CEWES MSRC are Computational Fluid Dynamics (CFD), Computational Structural Mechanics (CSM), Environmental Quality Modeling (EQM), Climate/Weather/Oceans Modeling (CWO), and Forces Modeling and Simulation (FMS).

Definitions of "Core Support" and "Focused Efforts" were developed in the revised PET plan for CEWES MSRC that was delivered to the government on 27 March 1997. This document provides detailed descriptions of PET team activities in Contract Year Three (April 1998 - March 1999). The academic partners associated with CEWES MSRC PET include: the Engineering Research Center (ERC) at Mississippi State University (MSU) (Lead University); the National Computational Science Alliance (NCSA) at the University of Illinois; the Center for Research in Parallel Computing (CRPC), led by Rice University and supported by the University of Tennessee at Knoxville (UTK) and the Northeast Parallel Architectures Center (NPAC) at Syracuse University; Jackson State University (Lead HBCU); Clark Atlanta University (HBCU); the Ohio Supercomputing Center (OSC) and the Ohio State University (OSU); the Texas Institute for Computational and Applied Mathematics (TICAM) at the University of Texas - Austin; and the University of Southern California (USC).

CORE SUPPORT

"Core Support" refers to that portion of PET that captures the minimum funding required for full-time positions and university leads. Significant lead time and funding assurance are required prior to university hiring commitments, so there needs to be some level of assurance that annual funding will be maintained at each university throughout the program. This, of course, does not preclude corrective action based on non-performance. PET staff activities at CEWES MSRC within Core Support include, but are not limited to:

- Providing High Performance Computing (HPC) training courses for MSRC users

- Providing a continual base of academic involvement in PET
- Ensuring greater freedom in the scope of university efforts
- Providing for longer duration academic efforts
- Administration of Training and Education Facility (TEF) operation and HPC training
- User outreach based on constant CTA utilization monitoring and taxonomy updates, user group participation, and one-on-one user assistance as required
- Assigned responsibilities for providing updated inputs to PET web pages and collaborative environments
- Regular reporting of activities/progress for each PET area
- SPP algorithm enhancement
  – Scalable parallelization fundamental issues
  – Development of **better numerics and science** for existing algorithms
- Integral PET role in Computational Migration
  – Support to specific key algorithm migrations as required
  – Identification of long-term algorithmic issues

The following Core Support efforts were approved for Year Two:

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- PET Leadership (Director, On-site Team Lead), Training Coordinator, SV On-site Lead (SAIC), Computational Migration support

Mississippi State University - ERC

- Academic Lead, CFD Lead and support team, CFD On-site Lead, CSM On-site Lead

NCSA - University of Illinois

- SV Lead and support team

CRPC - Rice/Tennessee/Syracuse

- **Rice University**
  - SPP Tools Lead and support team, SPP Tools On-site Lead
- **University of Tennessee**
  - SPP Tools support
- **NPAC - Syracuse University**
  - C/C Lead and support team, FMS Lead and support team, Training Lead and support team

Jackson State University

- HBCU/MI Lead and support team

Ohio State University / OSC

- Training support, CWO Lead and support team, Computational Migration support

TICAM - University of Texas

- EQM Lead and support team, EQM On-site Lead, CSM Lead and support team

Details of each Core Support effort are provided in Appendix A.

FOCUSED EFFORTS

"Focused Efforts" are activities funded by the remaining PET resources, which are allocated for approved "projects" based on PET team interactions with MSRC users and on proposals submitted by the university partners and approved by the PET leadership and CEWES MSRC. Focused Effort proposals are **evaluated** according to the following guidelines:

- Each proposed effort should be an HPC support activity related to national defense or national security.
- Proposed activity relevance to ongoing Common HPC Software Support Initiative (CHSSI) projects is considered.
- Extent to which effort complements MSRC hardware acquisition strategy is considered.
- Proposed effort relevance to ongoing DoD Challenge Projects is considered.
- Proposed effort exploitation of the Defense Research and Engineering Network (DREN) network capabilities is considered.
- Efforts should improve the effective utilization of HPC resources via
  - – Visualization and data interpretation
  - – Code performance enhancements
  - – Multi-architecture portability, etc.
- Proposed efforts should enhance the capability to use MSRC systems via
  - – Training and graduate courses
  - – HBCU/MI activities
  - – Collaborative environments, etc.

Obviously, every Focused Effort cannot meet all of these criteria, but they are used to judge the relevance and appropriate nature of proposals. Focused Efforts are **managed** according to the following rules:

- Authority to Proceed (ATP) is based on informal proposals submitted to the PET Director and the review/concurrence of PET leadership and the government
- Projects **must have** MSRC ***user advocacy and participation*** if at all possible

- Projects should have specific start and end dates, schedules, deliverables, budgets, and periodic progress reviews (every 3-6 months)
- Each effort is managed on a project-by-project basis (i.e., funding will be allocated on this basis)

The following Focused Efforts have been approved for Year Three:

Mississippi State University - ERC

- Visualization of Very Large Oceans Datasets
- Wavelet Based Multiresolutional Representation for CEWES MSRC datasets
- Tools Content for Educational CD-ROM
- Scalable and Parallel Integration of Hydraulic, Wave and Sediment Transport Models

NCSA - University of Illinois

- Interactive SV Computation
- Interactive SV Tools for EQM
- PET Web Pages Evolution

CRPC - Rice/Tennessee/Syracuse

- Inner Loop Analysis for HELIX Code (Rice)
- Evaluation of OpenMP as a Target for Code Migration (Rice)
- Tools Content for Educational CD-ROM (Rice)
- Real-time Interactive Performance Analysis and Debugging (UTK)
- Interoperable CTA Software Repositories II (UTK)
- MPI Interconnection and Process Management (UTK)
- High Performance Distributed Object Web based HLA Demonstration (NPAC)
- Web Interfaces for Computational Modules (NPAC)
- HPC Educational CD-ROM (NPAC)
- Distance Education for Curricula Enhancement (NPAC)
- Prototype Distance HPC Training for DoD Users (NPAC)

Jackson State University

- Web-Based Distance Education
- Scientific Visualization Lab

Clark Atlanta University

- Student Training
- Residual Capacity of Damaged Structures II
- Interpretation of Large Data Sets

Ohio State University/OSC

- Coupling Sediment, Circulation and Wave Models for Coastal Applications II (OSU)

- Parallelization of SED (OSU, joint with MSU)
- Prototype Distance HPC Training for DoD Users (OSC, joint with Syracuse)
- Support to CEWES MSRC Computational Migration Group (OSC)

TICAM - University of Texas

- A Coupled Hydrodynamic-Water Quality Model Based on ADCIRC3D and CE-QUAL-ICM
- An Example of Launching a Parallel Simulation Under the Groundwater Modeling System (GMS)
- Adaptive Mesh Technology Applied to Damaged Structures

University of Southern California

- Benchmarking HPC Systems II

Detailed descriptions of these Focused Efforts are provided in Appendix B.

The overall working theme for CEWES MSRC is "Scalable HPC Applications and Performance." Within the context of this "umbrella," PET is supporting a number of sub-themes, including scalable computing migration, HPC training and DoD user productivity, HPC performance metrics and tools, management and interpretations of large data sets, SV of very large (terabyte scale) problems, and DoD Challenge applications. The PET Core Support and Focused Efforts support the overall CEWES MSRC theme and sub-themes.

A complete list of current PET points of contact is provided in Appendix C.

Appendix A: Detailed Core Support Descriptions

1. Core Support Area: Academic Lead

Lead: Dr. Joe Thompson (MSU-ERC)

PI EMail Address: joe@erc.msstate.edu

PI Telephone: (601) 325-7299 **PI Fax:** (601) 325-7692

Statement of Work: MSU-ERC will provide a core level of effort to support the academic leadership of the PET program at CEWES MSRC. Responsibilities include, but are not limited to, participation the Academic Executive Committee (ExComm) for PET across the four MSRCs; maintaining knowledge of current status of all Focused Efforts ongoing at the (currently) ten participating university partners; reporting on status of Focused Efforts on a monthly basis; review and recommendations for funding of PET Focused Efforts; and participation in planning and execution of PET meetings (Mid-Year Review, Annual Review, workshops, DoD Users Meeting, etc.) as appropriate. MSU-ERC will select and attend conferences and other meetings that have high payoff and direct application for the PET program.

Deliverables:

- Trip reports for conferences and user contacts (as conducted)
- Conduct two MPI training classes at CEWES MSRC or remote user locations (as requested)
- Contributions to PET bi-weekly and Annual reports (every two weeks according to schedule and March 1999), including monthly reports on individual Focused Efforts

2. Core Support Area: Computational Fluid Dynamics (CFD)

Lead: Dr. David Huddleston (MSU-ERC)

PI EMail Address: hudd@erc.msstate.edu

PI Telephone: (601) 325-7193 **PI Fax:** (601) 325-7692

Statement of Work: MSU-ERC will provide a core level of effort to support the CFD on-site position for the PET program at CEWES MSRC. MSU will provide a core level of effort to support technology transfer, user outreach, training, and assessment of targeted codes and algorithms in CFD. Targeted codes include, but are not limited to, the CFD CHSSI codes, user codes, etc. Technology of interest includes, but is not limited to, grid generation codes, parallelization of CFD algorithms, numerical solvers, management and interpretation of large data sets, adaptive and meshless techniques, etc. MSU will maintain frequent contact with the DoD CTA Lead for CFD. MSU will select and attend focused conferences and other meetings that have high payoff and direct application for user interaction and technology transfer.

Deliverables:

- Trip reports for conferences and user contacts (as conducted)
- Contributions to PET bi-weekly and Annual reports (every two weeks according to schedule and March 1999), including monthly reports on individual Focused Efforts
- Presentations for PET Mid-Year and Annual Reviews (August 1998, January 1999)
- Contributions to PET website for CFD as appropriate

3. Core Support Area: Computational Structural Mechanics (CSM) -- MSU

Lead: Dr. Joe Thompson (MSU-ERC)

PI EMail Address: joe@erc.msstate.edu

PI Telephone: (601) 325-7299 **PI Fax:** (601) 325-7692

Statement of Work: MSU-ERC will provide a core level of effort to support the CSM on-site position for the PET program at CEWES MSRC. MSU will provide a core level of effort to support technology transfer, user outreach, training, and assessment of targeted codes and algorithms in CSM. Targeted codes include, but are not limited to, EPIC, CTH, DYNA3D, and NASTRAN. Technology of interest includes, but is not limited to, grid generation codes, management and interpretation of large (terascale) data sets, adaptive and meshless techniques, etc. MSU will maintain frequent contact with the DoD CTA Lead for CSM, to understand the priorities and ongoing CHSSI activities, as well as with Dr. Raju Namburu, the CEWES lead for CSM. MSU will select and attend focused conferences and other meetings that have high payoff and direct application for user interaction and technology transfer.

Deliverables:

- Trip reports for conferences and user contacts (as conducted)
- Contributions to PET bi-weekly and Annual reports (every two weeks according to schedule and March 1999), including monthly reports on individual Focused Efforts
- Presentations for PET Mid-Year and Annual Reviews (August 1998, January 1999)
- Contributions to PET website for CSM as appropriate

4. Core Support Area: Scientific Visualization (SV)

Lead: Dr. Polly Baker (NCSA-Illinois)

PI EMail Address: baker@ncsa.uiuc.edu

PI Telephone: (217) 244-1997 **PI Fax:** (217) 244-2909

Statement of Work: NCSA will provide a core level of effort (1.2 FTEs) to support technology transfer, user outreach, training, and assessment of targeted codes and algorithms in SV. Targeted codes include, but are not limited to, the Visualization ToolKit (VTK), AVS Express, PV3, CUMULVS, DICE, and possibly others. Technology of interest includes, but is not limited to, SV file formats (e.g., HDF), remote visualization, collaborative visualization, SV of highly multivariate problems, interactive steering, and use of multimodal indicators. NCSA will maintain frequent contact with Dr. Richard Strelitz (SAIC), the CEWES MSRC PET on-site Lead for SV, to facilitate technology transfer, user outreach, and relevance to current MSRC issues. Dr. Strelitz will provide the interface to the MSRC SV Center. Dr. Alan Shih, the at-NCSA team leader for SV, will spend 25% - 40% of his time at CEWES MSRC or at remote sites working with users of the center and with Dr. Strelitz.

NCSA will select and attend focused conferences and other meetings that have high payoff and direct application for user interaction and technology transfer. For each conference attended, NCSA will submit in advance a "statement of benefits" to PET that allows the NRC management to determine whether CEWES MSRC PET funding should be used to cover the cost of that meeting. Targeted training includes, but is not limited to, SV tools (VTK, AVS Express), an SV Workshop in the fall of 1998, etc. Such training may be conducted either at CEWES MSRC or at remote user sites as deemed necessary and appropriate. It may also include web-based tutorials as funding permits.

Deliverables:

- Trip reports for conferences and user contacts (as conducted)
- Contributions to PET bi-weekly and Annual reports (every two weeks according to schedule and March 1999)
- Presentations for PET Mid-Year and Annual Reviews (August 1998, January 1999)
- Training course materials (as conducted)
- All developed tools to be delivered to Dr. Strelitz for installation at the CEWES MSRC SVC
- Contributions to SV portion of CEWES PET website (as required)

5. Core Support Area: Scalable Parallel Programming (SPP) Tools -- Rice

Lead: Dr. Charles Koelbel (Rice)

PI EMail Address: chk@cs.rice.edu

PI Telephone: (713) 285-5304 **PI Fax:** (713) 285-5136

Statement of Work: Rice will provide a 1.5 FTE core level of effort to support technology transfer, user outreach, and training in SPP Tools. Technology of interest includes, but is not limited to, parallel debugging tools, parallel libraries, and vector to parallel conversion tools. Rice will maintain frequent contact with Dr. Clay Breshears, the CEWES MSRC PET on-site Lead for SPP Tools, to facilitate technology transfer, user outreach, and relevance to current MSRC issues.

Rice will select and attend focused conferences and other meetings that have high payoff and direct application for user interaction and technology transfer. For each conference attended, Rice will submit in advance a "statement of benefits" to PET that allows the NRC management to determine whether CEWES PET funding should be used to cover the cost of that meeting. Targeted training includes, but is not limited to, SPP tools, use of parallel tools and libraries, etc. Such training may be conducted either at CEWES MSRC or at remote user sites as deemed necessary and appropriate. Rice will continue to sponsor meetings of the HPCMP-wide Academic Executive Committee. This year's core support includes funding for Rice to conduct the June 1998 DoD Users Meeting.

Rice will continue its leadership of the PET Academic Executive Committee. This will include frequent teleconferences and meetings (in conjunction with other DoD-sponsored events such as the Users Group Meeting). It will also include maintenance of the ExComm website located at http://www.crpc.rice.edu/DODmod/.

Deliverables:

- Trip reports for conferences and user contacts (as conducted)
- Contributions to PET bi-weekly and Annual reports (every two weeks according to schedule and March 1999)
- Presentations for PET Mid-Year and Annual Reviews (August 1998, January 1999)
- Training course materials (as conducted)
- Contributions to SPP Tools portion of CEWES PET website
- Maintain PET ExComm website

6. Core Support Area: Scalable Parallel Programming (SPP) Tools -- UTK

Lead: Dr. Shirley Browne (Tennessee)

EMail Address: browne@cs.utk.edu

Telephone: (423) 974-3547 **Fax:** (423) 974-8296

Statement of Work: Tennessee will provide a core level of effort to support technology transfer, user outreach, and training in SPP Tools. Technology of interest includes, but is not limited to, parallel debugging tools, parallel libraries, and vector to parallel conversion tools. Tennessee will maintain frequent contact with Dr. Clay Breshears (Rice), the CEWES MSRC PET on-site Lead for SPP Tools, to facilitate technology transfer, user outreach, and relevance to current MSRC issues.

Tennessee will select and attend focused conferences and other meetings that have high payoff and direct application for user interaction and technology transfer. For each conference attended, Tennessee will submit in advance a "statement of benefits" to PET that allows the NRC management to determine whether CEWES PET MSRC funding should be used to cover the cost of that meeting. Targeted training includes, but is not limited to, SPP tools, use of parallel tools and libraries, etc. Such training may be conducted either at CEWES MSRC or at remote user sites as deemed necessary and appropriate and within budget constraints.

Deliverables:

- Trip reports for conferences and user contacts (as conducted)
- Contributions to PET bi-weekly and Annual reports (every two weeks according to schedule and March 1999)
- Presentations for PET Mid-Year and Annual Reviews (August 1998, January 1999)
- Contributions to SPP Tools portion of CEWES PET website

7. Core Support Area: Forces Modeling and Simulation/C4I (FMS)

Lead: Dr. David Bernholdt (NPAC-Syracuse)

PI EMail Address: bernhold@npac.syr.edu

PI Telephone: (315) 443-3857 **PI Fax:** (315) 443-1973

Statement of Work: Syracuse will provide a core level of effort to support technology transfer, user outreach, training, and assessment of targeted codes and algorithms in FMS. Targeted codes include, but are not limited to, the Comprehensive Mine Simulator (CMS), Modular Simulation of Armed Forces (ModSAF), and SPEEDES. Technology of interest includes, but is not limited to, High-Level Architecture (HLA) simulations, CORBA and Java-based Run-Time Infrastructure (RTI), and other concepts being implemented by joint DoD simulation efforts. Syracuse will maintain frequent contact with the DoD CTA Lead for FMS, to understand the priorities and ongoing CHSSI activities. Syracuse will select and attend focused conferences and other meetings that have high payoff and direct application for user interaction and technology transfer. Targeted training includes, but is not limited to, distributed computing, Java, Object Web RTI, etc. Such training may be conducted either at CEWES MSRC or at remote user sites as deemed necessary and appropriate.

Deliverables:

- Trip reports for conferences and user contacts (as conducted)
- Contributions to PET bi-weekly and Annual reports (every two weeks according to schedule and March 1999)
- Presentations for PET Mid-Year and Annual Reviews (August 1998, January 1999)
- Training course materials (as conducted)
- Develop and maintain a web site describing FMS activities of interest to CEWES MSRC users.

Notes: Syracuse should work with Dr. Wayne Mastin to identify and target at least one opportunity to conduct FMS training during Year Three.

8. Core Support Area: Collaboration/Communication (C/C)

Lead: Dr. David Bernholdt (NPAC-Syracuse)

PI EMail Address: bernhold@npac.syr.edu

PI Telephone: (315) 443-3857 **PI Fax:** (315) 443-1973

Statement of Work: Syracuse will provide a core level of effort to support technology transfer, user outreach, training, and assessment of tools and technologies to facilitate communication and collaboration among the PET team and users of the CEWES MSRC. Technologies of interest include, but are not limited to, both synchronous and asynchronous collaboration over the Internet and use of databases to manage large volumes of information, especially when coupled with web servers to facilitate access to the information. Syracuse will provide an appropriate level of effort to support the deployment and use of the Tango collaboratory tool, emphasizing robustness and core collaboration functionality. Syracuse will continue to operate and enhance web-linked database applications it has developed for CEWES MSRC, and, as requested, assist with transfer to on-site computer systems. Syracuse will maintain frequent contact with CEWES MSRC Webmasters, database administrators, and other on-site personnel to insure that C/C resources provide the maximum utility to the PET/user community. Syracuse will also maintain regular contact with PET team members to assess needs. Syracuse will select and attend focused conferences and other meetings that have high payoff and direct application for team and user interaction and technology transfer.

Deliverables:

- Trip reports for conferences and user contacts (as conducted)
- Contributions to PET bi-weekly and Annual reports (every two weeks according to schedule and March 1999)
- Presentations for PET Mid-Year and Annual Reviews (August 1998, January 1999)
- On-going enhancement of the Tango in support of collaboration:
  - Tango 2 release with rewritten server and client for increased robustness (October 1998)
  - Tango 2 release with linkage to database, including Lotus Notes, for asynchronous collaboration (January 1999)
- On-going Operation and enhancement of web-linked database applications
- Assistance with transfer of web-linked database applications to CEWES MSRC computer systems (TBD)
- Training on web-linked database technology (TBD)

- Tango training at 27 April 1998 NCSA Alliance meeting and 26-27 June 1998 national meeting on web-based education and training in San Diego (DoD personnel will be invited to both events)
- Develop and maintain a web site with information on C/C tools and technologies

9. Core Support Area: Training

Lead: Dr. David Bernholdt (NPAC-Syracuse)

EMail Address: bernhold@npac.syr.edu

Telephone: (315) 443-3857 **Fax:** (315) 443-1973

Statement of Work: Syracuse will provide a core level of effort to support technology transfer, user outreach, and long-range leadership on issues of technology, tools, and techniques related to PET Training and Educational needs. Technologies of interest include, but are not limited to, synchronous and asynchronous web/Internet-based distance education tools, electronic repositories of training materials, etc. Of particular, but not exclusive, interest are the Tango and WebWisdom systems developed by Syracuse. Syracuse will provide an appropriate level of effort to support these tools, as they are used in a variety of PET-supported educational and training projects, emphasizing the general robustness of the tools. Syracuse will maintain frequent contact with the on-site Training team at the CEWES MSRC to understand the needs and use of training technology at the MSRC. Syracuse will also be active in meetings of the PET Program-Wide Training Group, especially in monitoring and advising on the program-wide deployment of tools and technologies. Syracuse will select and attend focused conferences and other meetings that have high payoff and contribute directly to providing leadership on training technology issues.

Deliverables:

- Trip reports for conferences and user contacts (as conducted)
- Contributions to PET bi-weekly and Annual reports (every two weeks according to schedule and March 1999)
- Presentations for PET Mid-Year and Annual Reviews (August 1998, January 1999)
- Involvement in PET Program-Wide Training Group meetings and activities (as conducted)
- On-going enhancement of the Tango and WebWisdom in support of education and training activities:
  - Tango 1.0 release with packaged NT and UNIX servers and web sites. Full support for all browsers (May 1998)
  - Tango 2 release with rewritten server and client for increased robustness (October 1998)
- Contribute materials pertaining to education and training technologies to the CEWES MSRC PET Training web site
- Evaluation of multimedia database needs for training materials (July 1998)

10. Core Support Area: HPC Support to HBCUs/MIs

Lead: Dr. Willie Brown

EMail Address: wbrown@ccaix.jsums.edu

Telephone: (601) 968-2105 **Fax:** (601) 968-2478

Statement of Work: In cooperation with NPAC-Syracuse and NCSA, JSU will conduct focused activities in distance learning and education and in remote scientific visualization. JSU will maintain constant contact and interface with the Training Lead at Syracuse (Prof. Geoffrey Fox), the SV Lead at NCSA (Dr. Polly Baker), the Training Coordinator at CEWES MSRC (Mr. John Eberle), and the On-site SV Lead at CEWES MSRC (Dr. Richard Strelitz). JSU will identify specific efforts for students and staff to test and evaluate distance learning and remote visualization technologies in the facilities at the university. JSU will organize and sponsor a Summer Institute designed to provide an introduction to HPC technology to minority students at multiple institutions.

Deliverables:

- Trip reports for conferences and user contacts (as conducted)
- Contributions to PET bi-weekly and Annual reports (every two weeks according to schedule and March 1999)
- Presentations for PET Mid-Year and Annual Reviews (August 1998, January 1999)
- Final “pre-print” report describing progress in evaluating and using distance learning and remote visualization technologies (Mar 99)
- Contributions to HBCU portion of CEWES PET website

11. Core Support Area: Climate / Weather / Oceans (CWO) Modeling

Lead: Drs. Keith Bedford and P. Sadayappan (OSU)

PI EMail Address: bedford.1@osu.edu, sadayappan.1@osu.edu

PI Telephone: (614) 292-7338 **PI Fax:** (614) 292-3780

Statement of Work: OSU will provide a core level of effort to support technology transfer, user outreach, training, and assessment of targeted codes and algorithms in CWO. Targeted codes include, but are not limited to, WAM, CH3D, SWAN, SED and COSED. Technology of interest includes, but is not limited to, application of circulation and wave models to sea condition prediction, coupling of wave, sediment and circulation models, etc. OSU will maintain frequent contact with the DoD CTA Lead for CWO, to understand the priorities and ongoing CHSSI activities, as well as with Dr. Robert Jensen, the local CWO representative at CEWES. OSU will select and attend focused conferences and other meetings that have high payoff and direct application for user interaction and technology transfer. Targeted training includes, but is not limited to, participation in the JSU Summer Institute (June 1998) and a possible CWO workshop in February 1999. Dr. David Welsh, who will spend between 25% and 40% of his time at CEWES MSRC during the contract year.

Deliverables:

- Trip reports for conferences and user contacts (as conducted)
- Contributions to PET bi-weekly and Annual reports (every two weeks according to schedule and March 1999)
- Presentations for PET Mid-Year and Annual Reviews (August 1998, January 1999)
- Training course materials (as conducted)
- Contributions to web site describing CWO activities of interest to CEWES MSRC users.

12. Core Support Area: Environmental Quality Modeling (EQM)

Lead: Dr. Mary Wheeler (TICAM-Texas)

PI EMail Address: mfw@ticam.utexas.edu

PI Telephone: (512) 475-8625 **PI Fax:** (512) 471-8694

Statement of Work: Texas will provide a core level of effort to support technology transfer, user outreach, and training in EQM. Technology of interest includes, but is not limited to, groundwater modeling, parallel partitioning methods, numerical solvers, etc. Texas will maintain frequent contact with Dr. Robert Fithen, the CEWES PET on-site Lead for EQM, to facilitate technology transfer, user outreach, and relevance to current MSRC issues. Targeted codes include, but are not limited to, 3D-ADCIRC, parallel CE-QUAL-ICM, and FEMWATER.

Texas will select and attend focused conferences and other meetings that have high payoff and direct application for user interaction and technology transfer. For each conference attended, Texas will submit in advance a "statement of benefits" to PET that allows the NRC management to determine whether CEWES PET funding should be used to cover the cost of that meeting. Targeted training includes, but is not limited to, a Workshop on Parallel Algorithms and a Workshop on Parallel Technology. Such training may be conducted either at CEWES MSRC or at remote user sites as deemed necessary and appropriate

Deliverables:

- Trip reports for conferences and user contacts (as conducted)
- Contributions to PET bi-weekly and Annual reports (every two weeks according to schedule and March 1999)
- Presentations for PET Mid-Year and Annual Reviews (August 1998, January 1999)
- Training course materials (as conducted)
- Contributions to EQM portion of CEWES PET website

13. Core Support Area: Computational Structural Mechanics (CSM) -- Texas

Lead: Dr. Tinsley Oden (TICAM-Texas)

PI EMail Address: oden@ticam.utexas.edu

PI Telephone: (512) 471-3312 **PI Fax:** (512) 471-8694

Statement of Work: TICAM will provide a core level of effort to support technology transfer, user outreach, and training. Technology of interest includes, but is not limited to, adaptive mesh and grid algorithms and tools, management of large CSM data sets, and parallelization/coupling of key CSM codes. Texas will maintain regular contact with Dr. Richard Weed, the CEWES MSRC PET on-site Lead for CSM, to facilitate technology transfer, user outreach, and relevance to current MSRC issues. Related codes include CTH, DYNA3D and EPIC. During the year, TICAM will make periodic visits to CEWES MSRC to work with the DoD users and on-site personnel for CSM.

TICAM will select and attend focused conferences and other meetings that have high payoff and direct application for user interaction and technology transfer. For each conference attended, Texas will submit in advance a "statement of benefits" to PET that allows the NRC management to determine whether CEWES MSRC PET funding should be used to cover the cost of that meeting. Targeted training includes, but is not limited to, training courses/workshops on grid generation, adaptive grids, management of large data sets, and efficient reliable HPC computations. Such training may be conducted either at CEWES MSRC or at remote user sites as deemed necessary and appropriate. TICAM will work with the On-site Team Lead to arrange at least two training classes during the year.

Deliverables:

- Lectures at DoD Users Meeting, Houston (June 1998)
- Trip reports for conferences and user contacts (as conducted)
- Contributions to PET bi-weekly and Annual reports (every two weeks according to schedule and March 1999)
- Presentations for PET Mid-Year and Annual Reviews (August 1998, January 1999)
- Training course materials (as conducted)
- Contributions to CSM portion of CEWES PET website

Appendix B: Detailed Focused Effort Descriptions

1. Focused Effort Title: Visualization of Very Large Oceans Datasets

Thematic Area(s): SciVis for Very Large Problems

PI Name: Dr. Robert Moorhead (MSU-ERC)

PI EMail Address: rjm@erc.msstate.edu

PI Telephone: (601) 325-2850 **PI Fax:** (601) 325-7692

Statement of Work: ERC will add CEWES/MSRC data readers and appropriate visualization mappings to a suite of visualization tools developed at MSU. The toolkit is called EnVis and presently consists of a batch-mode movie-making toolkit and an interactive visualization system. EnVis utilizes the OpenInventor library and is written in C++. Week long visits every other month to CEWES MSRC will provide the opportunity to understand various scientists' problems and to teach people how to use both the ERC systems and other systems within CEWES MSRC.

Most computational scientists would like to make a movie of computed output every night and use an interactive visualization system to look at about 5% of these results in greater detail and/or depth. Thus making a batch mode movie is a necessary preliminary step to encourage most model developers to use an interactive system. Most model developers are only interested in exploring their data in a virtual environment for about 1% of their model results. One benefit is the ability to tailor a visualization system to the needs of the particular discipline or problem, without having to write a completely new system. Exploiting modularity and plug-ins allows the scientist to include only the routines she/he wants/needs. This system will allow the novice user to use the visualization resources of the MSRC more effectively. The hands-on training will help people visualize their data more effectively. An understanding of wave heights and surf zones is a CWO data issue highly relevant to national defense. Understanding coastal and estuary flow patterns is crucial to national security. Visualization allows us to exploit the best pattern recognition and analysis toolset known -- our eyes and brain. There are many ongoing CHSSI projects which could benefit from better visualization tools, including WAM.

Deliverables:

- Deliver and install EnVis evMovieLoop2D, evMovieLoop3D, evInteractive2D, and evInteractive3D (May 1998)
- Demonstrate capability of tools to jointly-targeted potential users in CWO, CFD and EQM (September 1998)
- Contributions to PET bi-weekly and Annual reports (every two weeks according to schedule and March 1999)

- Presentations for PET Mid-Year and Annual Reviews (August 1998, January 1999)
- Assist at least two CEWES MSRC users in producing SV products from ERC tools (January 1999)
- "Pre-print" report on results of effort (March 1999)

2. Focused Effort Title: Wavelet Based Multiresolutional Representation for CEWES MSRC datasets

Thematic Area(s): SciVis for Very Large Problems

PI Name: Dr. Raghu Machiraju (MSU-ERC)

PI EMail Address: raghu@erc.msstate.edu

PI Telephone: (601) 325-2758 **PI Fax:** (601) 325-7692

Statement of Work: Concurrent (evolving simulations) and retrospective (post-processing) visualization are being used to monitor, verify and validate the results of various numerical simulations through large archival scientific databases. The generated datasets are large in size and are sampled usually on irregularly spaced grids (structured and unstructured). There exists a need for representation schemes which allow efficient feature extraction and region-of-interest extraction, such as: shocks, vortices; consideration of a multitude of grids; and access of structures in an increasing order of smoothness (or decreasing order of significance). To that end, ERC will pursue an approach based on wavelet analysis and intelligent feature detection/extraction that will operate effectively across both low and high bandwidth networks. This project addresses multiresolutional representation of datasets arising from a computational field simulation (e.g. wave modeling, sediment transport, etc.). The mainstay of this effort is the wavelet transform, which has been shown to be useful for analysis and compression of datasets. The approach determines the regions of interest by performing a feature detection exercise, breaks the volume into variable size blocks to localize the information, and then codes each block using a wavelet transform. The blocks are then ranked by visual information content so that the most informative wavelet coefficients can be embedded in a bitstream for progressive transmission or access. ERC will pursue this effort in cooperation with an NCSA effort to use CUMULVS to access the large data outputs of the CTH code.

Deliverables:

- Detailed briefing on application of this methodology to CTH data (May 1998)
- Demonstrate application to CTH (September 1998)
- Contributions to PET bi-weekly and Annual reports (every two weeks according to schedule and March 1999)
- Presentations for PET Mid-Year and Annual Reviews (August 1998, January 1999)
- Full demo of application to CTH and at least one other CEWES MSRC user code (January 1999)
- "Pre-print" report on results of effort (March 1999)

3. Focused Effort Title: Tools Content for Educational CD-ROM

Thematic Area(s): HPC Training and DoD User Productivity

PI Names: Dr. Joe Thompson (MSU-ERC)

PI EMail Address: joe@erc.msstate.edu

PI Telephone: (601) 325-7299 **PI Fax:** (601) 325-7692

Statement of Work: MSU will provide educational materials to Syracuse on MPICH, MPIX, and MPI++ for the CD-ROM that NPAC is producing for CEWES MSRC.

Deliverables:

- Educational materials delivered to Syracuse (September 1998)

4. Focused Effort Title: Scalable and Parallel Integration of Hydraulic, Wave and Sediment Transport Models

Thematic Area(s): Scalable Computing Migration

PI Name: Drs. Jianping Zhu and David. H. Huddleston (MSU-ERC)

PI EMail Address: jzhu@erc.msstate.edu, hudd@erc.msstate.edu

PI Telephone: (601) 325-7299 **PI Fax:** (601) 325-7692

Statement of Work: The DoD has been using separate wave (WAM), hydraulic (CH3D) and sediment transport (SED and COSED) models to conduct simulations for various applications. These studies are performed in direct support of DoD military operations, such as navigation and amphibious landings, as well as civil works projects important to DoD missions. High fidelity, large-scale simulations to provide improved operational and design decisions necessitate the integration of all three of these models. This effort will supplement the work conducted within CWO pertaining to a related topic. It will focus on the scalable and parallel integration of a cohesive sediment transport model into the hydraulic model, and collaboration with CWO and EQM groups for the integration of the wave model. This effort will build on earlier CFD PET support which led to the initial parallelization of CH3D. The sediment transport codes (SED and COSED) will be analyzed and parallelized within the hydrodynamic model. Verification of this initial parallel version will be completed. Integration with the wave model will be coordinated with the CWO and EQM groups. The parallel implementation will be accomplished using MPI to ensure maximum portability to different computing platforms.

Deliverables:

- Code acquisition and analysis (May 1998)
- Complete analysis and initiation of parallelization (September 1998)
- Contributions to PET bi-weekly and Annual reports (every two weeks according to schedule and March 1999)
- Presentations for PET Mid-Year and Annual Reviews (August 1998, January 1999)
- Initial parallelization complete (January 1999)
- Verification and benchmarking for the initial parallel implementation and "Pre-print" report on results of effort (March 1999)

5. Focused Effort Title: Interactive SV Computation

Thematic Area(s): SciVis for Very Large Problems

PI Name: Dr. Polly Baker (NCSA-Illinois)

PI EMail Address: baker@ncsa.uiuc.edu

PI Telephone: (217) 244-1997 **PI Fax:** (217) 244-2909

Statement of Work: NCSA will assess the applicability of multiple co-processing systems to CEWES MSRC user requirements, including but not limited to: CUMULVS, DICE, PV3, scivis, SCIRun, etc. An initial assessment will be made to CEWES MSRC PET management at the end of two months. At that time, NCSA will recommend one or more specific example applications (e.g., integration of CTH with CUMULVS or PV3 with CE-QUAL-ICM) to demonstrate co-processing using an actual CEWES MSRC user code. Subsequent work will involve integrating these tools and reporting on this experience. A final report will be delivered with recommendations on selecting appropriate co-processing systems.

In addition, NCSA will assess the applicability of their Hierarchical Data Format (HDF) to CEWES MSRC user visualizations. They will offer a seminar or training session on HDF for presentation at CEWES MSRC during the second quarter of Year Three.

Deliverables:

- Presentation to CEWES MSRC on co-processing systems (June 1998)
- Contributions to PET bi-weekly and Annual reports (every two weeks according to schedule and March 1999)
- Demonstration of co-processing with example application (September 1998)
- Presentations for PET Mid-Year and Annual Reviews (August 1998, January 1999)
- Mid-year report on experience with using each tool (October 1998)
- Final "pre-print" report with guidelines for tool selection (March 1999)
- All developed tools to be delivered to Dr. Strelitz for simultaneous installation at the CEWES MSRC SVC

6. Focused Effort Title: Interactive SV Tools for EQM

Thematic Area(s): SciVis for Very Large Problems

PI Name: Dr. Polly Baker (NCSA-Illinois)

PI EMail Address: baker@ncsa.uiuc.edu

PI Telephone: (217) 244-1997 **PI Fax:** (217) 244-2909

Statement of Work: NCSA will upgrade VisGen, the VTK-based tool prototyped and delivered to CEWES MSRC in Year Two. Specifically, the tool will be customized to meet the needs of the Chesapeake Bay "scenario" runs. This will include support for long duration runs, automated production of animations, non-interpolated color coding of cells, display of normalized cells, and switching between normalized and computational cells. NCSA will also extend the types of data that VisGen can read in order to extend the tool's usefulness beyond CE-QUAL-ICM users. The final CEWES MSRC customization of this tool will be delivered in August 1998, with user documentation.

Deliverables:

- Delivery of upgraded VTK tool (May 1998)
- Contributions to PET bi-weekly and Annual reports (every two weeks according to schedule and March 1999)
- Presentations for PET Mid-Year and Annual Reviews (August 1998, January 1999)
- Final delivery of CEWES MSRC customized tool and final "pre-print" report (August 1998)
- All developed tools to be delivered to Dr. Strelitz for simultaneous installation at the CEWES MSRC SVC

7. Focused Effort Title: PET Web Pages Evolution

Thematic Area(s): HPC Training and DoD User Productivity

PI Name: Sandie Kappes (NCSA-Illinois)

PI EMail Address: skappes@ncsa.uiuc.edu

PI Telephone: (217) 244-2170 **PI Fax:** (217) 244-2909

Statement of Work: NCSA will continue to evolve the structure of the CEWES MSRC PET web pages. They will work directly with the MSRC webmaster and cooperate with complementary Collaboration/ Communication efforts underway at NPAC-Syracuse. In addition, NCSA will provide support to the currently installed netWorkPlace collaborative software.

Deliverables:

- Contributions to PET bi-weekly and Annual reports (every two weeks according to schedule and March 1999)
- Presentations for PET Mid-Year and Annual Reviews (August 1998, January 1999)
- All developed software to be delivered to the CEWES MSRC Webmaster
- Final "pre-print" report on effort due on or before 31 Mar 99

8. Focused Effort Title: Inner Loop Analysis for HELIX Code

Thematic Area(s): Scalable Computing Migration

PI Names: Drs. Ehtesham Hayder, Gina Goff, Chuck Koelbel (Rice)

PI EMail Address: hayder@cs.rice.edu

PI Telephone: (713) 285- 5868 **PI Fax:** (713) 285-5136

Statement of Work: HELIX is a CFD code to solve unsteady full potential equations in the Eulerian grid with an embedded vortical velocity that models the influence of the wake. This code is used to compute compressible rotor flow fields in hover and forward flight with free wake. Such results can be used to calculate vibratory air loads in forward flight and the performance in hover. At present, HELIX is being ported to parallel machines at CEWES MSRC. The performance of the parallel version depends on how well it is mapped to the underlying computer architecture. It is suspected now that implementations in the present version of the parallel code do not utilize registers efficiently, resulting in poor speed-ups. Of particular concern is the performance of the "inner" loops in the FORTRAN code. Many implementation bottlenecks can be removed by changing how the code is written. Rice will examine how performance of the present version can be improved by changing its structure, and identify any weaknesses of the FORTRAN compiler. The goal is to reduce execution times of the code and to provide a detailed analysis of the inner loop performance in FORTRAN.

Deliverables:

- Identify critical sections and inner loops in HELIX code (July 1998)
- Analysis of inner loops and other critical sections of the HELIX code by advanced compilation techniques (September 1998)
- Delivery of inner loop analysis and improve implementation of the HELIX code (February 1999)
- "Pre-print" report on results of effort (March 1999)

9. Focused Effort Title: Evaluation of OpenMP as a Target for Code Migration

Thematic Area(s): Scalable Computing Migration

PI Names: Dr. Gina Goff (Rice)

PI EMail Address: gina@cs.rice.edu

PI Telephone: (713) 527-8750, X2732 **PI Fax:** (713) 285-5136

Statement of Work: Directives have frequently been used to implement parallelization on shared memory machines, but the nature of the directives has varied from one vendor to another, hindering the portability of application programs. OpenMP is a recently proposed standard that consolidates those directives into a single syntax and semantics. Apart from the obvious appeal of porting an application to a new machine without changing directives, OpenMP allows verifiable correctness of parallel programs. Correctness is vital to a wide range of DoD applications, where the consequences of an incorrect parallelization can be serious. Directives can also be easier for many programmers to understand and implement than either threads or message passing, an important consideration when codes are large, complex, or maintained by a succession of users. OpenMP provides scalability by supporting coarse grain parallelism through the use of directives that permit information needed to parallelize a loop or subroutine to appear anywhere in the program, instead of requiring its presence in the subroutine, making it easier to write complex codes and use parallelized libraries. There are also directives that allow the user to divide work up among threads. Several major hardware and software vendors are developing OpenMP products, ensuring its support on multiple platforms and operating systems

Rice will evaluate software related to OpenMP, on kernels representative of DoD codes to determine whether CEWES MSRC users can profitably exploit it. In particular, a beta version of the next release of SGI's F90 compiler, which supports OpenMP directives, has been installed on the Origin 2000. In addition, Kuck and Associates currently market a collection of OpenMP tools for a variety of machines. Their KAP/Pro Toolset includes software to aid application conversion, provide performance evaluation, and test programming correctness. Such tools could provide invaluable assistance to users trying to migrate codes to the Origin 2000. If time and funding permit, Rice will evaluate more advanced problems in OpenMP such as interfacing with MPI and HPF.

Deliverables:

- Contributions to PET bi-weekly and Annual reports (every two weeks according to schedule and March 1999)

- Presentations for PET Mid-Year and Annual Reviews (August 1998, January 1999)
- Evaluation of OpenMP as applied to sections of programs of interest to CEWES MSRC (October 1998)
- "Pre-print" report describing application of OpenMP to programs of interest to CEWES MSRC (March 1999)

10. Focused Effort Title: Tools Content for Educational CD-ROM

Thematic Area(s): HPC Training and DoD User Productivity

PI Names: Dr. Chuck Koelbel (Rice)

PI EMail Address: chk@cs.rice.edu

PI Telephone: (713) 285-5304 **PI Fax:** (713) 285-5136

Statement of Work: Rice will provide educational materials to Syracuse on Designing and Building Parallel Programs and High Performance FORTRAN for the CD-ROM that NPAC is producing for CEWES MSRC.

Deliverables:

- Educational materials delivered to Syracuse (September 1998)

11. Focused Effort Title: Real-time Interactive Performance Analysis and Debugging

Thematic Area(s): HPC Performance Metrics/Tools, HPC Training and DoD User Productivity

PI Name: Dr. Shirley Browne (Tennessee)

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PI Telephone: (423) 974-3547 **PI Fax:** (423) 974-8296

Statement of Work: This project is a continuation of Tennessee's Year Two "Parallel Performance and Debugging Tools" focused effort. Tennessee will continue the evaluation and deployment of trace-based performance tools begun in Year Two, but will add a new emphasis on real-time interactive analysis. Tennessee will continue to port, test, debug, and enhance selected trace-based tools for doing post-mortem performance analysis. These tools include AIMS, nupshot, and the various Pablo components. The Year Three project has three new components, each of which involves collaboration with other researchers on major performance analysis or debugging projects. The first two components target major DARPA-supported performance analysis research projects, with the goal of transferring the results of this research to DoD users.

The first component involves technology transfer of research results and prototype tools from the DARPA-supported Pablo performance analysis project at the University of Illinois to DoD users. Tennessee will focus on real-time analysis and visualization of application performance and analysis and tuning of I/O performance. The Pablo performance data capture tools can be operated in two modes, either writing the performance data to a trace file or sending performance data to a socket for real-time analysis. Tennessee will experiment with the second mode on DoD HPC platforms and with coupling the performance data output to Pablo analysis tools running on advanced visualization hardware such as the ImmersaDesk, as well as on more generally available workstations. This work will include installation, testing, and support of the new Pablo virtual environment toolkit, called Virtue, on the CEWES MSRC SVC systems. The Virtue system immerses the user in scalable, hierarchical representations of software structure and real-time performance data. Through coupled virtual environments, multiple, physically separated users will be able to collaboratively explore and manipulate the same software and performance data representations. Virtue is targeting applications drawn from both the embedded real-time domain and the large-scale scientific computing domain. This part of the project will involve collaboration with SV PET team members to obtain guidance on the most appropriate visualization systems and techniques to use for

visualizing application performance data. Tennessee will also collaborate with Jackson State University through a summer student intern who will work with them on this part of the project.

The second component involves collaboration with the Paradyn team at the University of Wisconsin on a dynamic instrumentation approach to performance analysis and debugging. The Paradyn tool, developed as part of a DARPA-funded project at Wisconsin, provides real-time interactive visualization of performance data for parallel programs, as well as an automatic, self-refining search for performance bottlenecks. The dyninst API used by Paradyn has been proposed by Douglas Pase of IBM as the basis for a more general client-server system, called the Dynamic Application Instrumentation System (DAIS), that will provide a portable dynamic instrumentation interface for developing portable debugging, performance analysis, and computational steering tools. Tennessee will collaborate with Wisconsin to develop versions of Paradyn that will work on the CEWES MSRC platforms. Tennessee will participate in the dyninst/DAIS standardization effort being led by Pase and will help test, debug, and interface tools to DAIS reference implementations on DoD platforms. The DOE ASCI Common Basic Environment (CBE) project, led by Jeff Brown at Los Alamos National Lab and with whom Tennessee will also collaborate, is also participating in the dyninst/DAIS effort.

The third component involves collaboration with Oregon State (PI Dr. Cherri Pancake) on the NAVO-funded PET effort to develop a reference implementation of the proposed High Performance Debugging version 1 standard for the IBM SP and Origin 2000. Oregon State will develop the front-end parser. Both the p2d2 system developed at NASA Ames and DAIS have been suggested as back ends. Tennessee will develop and implement the protocol that connects the front and back ends. In addition, Tennessee will conduct a usability study of debugging interfaces to obtain input from DoD users to guide the development of HPD version 2, which is expected to include graphical user interface and graphical data display specifications.

Deliverables: [Note: The following list of deliverables is over-subscribed and depends on the results of outside projects which may not come in on schedule, but Tennessee agrees to deliver opportunistically on items related to Pablo, HPD, Paradyn, Pablo Virtue, and DAIS.]

- Finish deployment and documentation of trace-based tools on CEWES MSRC platforms (May 1998)
- Experiment with Pablo real-time data capture module (May 1998)
- HPD reference implementation for IBM SP (July 1998)
- Modify Paradyn to work on CEWES MSRC platforms (in collaboration with Paradyn developers) (August 1998)

- Deploy and test Pablo Virtue system at CEWES MSRC (joint work with summer student intern from Jackson State) (August 1998)
- I/O characterization of DoD applications (collaboration with ASC and ARL-funded scalable I/O project at Jackson State) (August 1998)
- Test, debug, and experiment with DAIS implementation for IBM SP (expected to be made available June 98) (August 1998)
- Contributions to PET bi-weekly and Annual reports (every two weeks according to schedule and March 1999)
- Presentations for PET Mid-Year and Annual Reviews (August 1998, January 1999)
- HPD reference implementation for SGI Origin 2000 (November 1998)
- Test, debug, and experiment with DAIS implementation for SGI Origin 2000 (expected to be made available Sep 98) (November 1998)
- Performance evaluation of parallel I/O systems (November 1998)
- Experimental use of Paradyn and Virtue with selected CTAs (November 1998)
- Workshops on use of Virtue and Paradyn systems (January 1999)
- Couple DAIS server with Pablo analysis tools (March 1999)
- "Pre-print" report on results of effort (March 1999)
- Transfer cache performance measurement tool and tuning methodology developed under the DOE ASCI program to DoD users
- Work with the CEWES MSRC SVC to integrate performance data visualization with existing SV software

12. Focused Effort Title: Interoperable CTA Software Repositories II

Thematic Area(s): HPC Training and DoD User Productivity

PI Name: Dr. Shirley Browne (Tennessee)

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PI Telephone: (423) 974-3547 **PI Fax:** (423) 974-8296

Statement of Work: This effort is for a continuation of the Year Two effort with the same title. The DoD HPCMP effort will undoubtedly produce an abundance of software and other reusable assets. A system is needed whereby these assets can be archived and shared among the MSRCs, DCs, and other DoD sites and users. One system that can meet this need is the Repository in a Box (RIB) toolkit. Tennessee will apply RIB, with necessary extensions of its functionality, to set up a distributed collection of interoperable software repositories for the DoD HPCMP CTAs. This network of repositories will allow codes, algorithms, and experiences to be shared within and among CTAs. Use of RIB will provide a uniform and consistent user interface to these repositories. At SC97, Tennessee demonstrated an HPC software repository using the production installation of RIB at ASC MSRC and prototype installations at ARL MSRC and CEWES MSRC. With ASC MSRC funding, a CCM repository has been set up at ASC MSRC, and with ARL MSRC funding, CCM and SIP repositories are being set up at ARL MSRC. Tennessee has drawn up an initial classification scheme for CFD software and is ready to set up a CFD repository at CEWES MSRC and begin populating it. A new version of RIB that supports file uploading and automatic mirroring has recently been released.

For year 3, Tennessee will:

- continue development of the CFD repository
- implement a training materials repository that will contain current versions and updates to materials on the HPC Education CD-ROM being developed by Syracuse
- implement access control
- implement interoperation with other DoD and NHSE repositories
- develop additional software repositories in other areas

Deliverables:

- Identify and catalog available CFD software (May 1998)
- Identify access control and licensing requirements (May 1998)
- Implement access control and electronic licensing (August 1998)
- Implement training materials repository (September 1998)

- Contributions to PET bi-weekly and Annual reports (every two weeks according to schedule and March 1999)
- Presentations for PET Mid-Year and Annual Reviews (August 1998, January 1999)
- Establish a repository for one or more additional areas (possibly grid generation and EQM) (November 1998)
- Establish and interoperate with CFD repositories at other MSRCs (December 1998)
- Outreach to distributed centers and remote users (March 1999)
- "Pre-print" report on results of effort (March 1999)

13. Focused Effort Title: MPI Interconnection and Process Management

Thematic Area(s): Scalable Computing Migration, HPC Performance Metrics/Tools, DoD Challenge Applications

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PI Telephone: (423) 974-8295 **PI Fax:** (423) 974-8296

Statement of Work: This effort is a continuation of the Year Two project with the same title. The problem is that different vendors' MPI implementations cannot interoperate directly with one another. As a result, distributed computing using MPI across different vendors' machines, or even between two of the same parallel platforms, requires use of a heterogeneous MPI implementation, such as MPICH. This solution may be sub-optimal because it cannot utilize the vendors' own optimized MPI implementations. MPI-Connect (formerly called PVMPI), a software system under development at the University of Tennessee, provides the needed interoperability between different vendors' optimized MPI implementations. MPI-Connect is transparent to MPI applications in that it allows intercommunication between different MPI implementations (or instances of the same implementation on different machines) using normal MPI communication calls. Such calls are intercepted by MPI-Connect via the MPI profiling interface. If the communication is within the same machine, then the native MPI call is invoked with little overhead. Otherwise, MPI-Connect handles the communication on and off the machine. MPI-Connect will also provide some of the MPI-2 process control and parallel I/O features. To summarize, MPI-Connect has been successfully ported to and tested with vendor MPI on the IBM SP and SGI Origin 2000 platforms. Work has begun on the port to the Cray T3E. The Cray T3E port requires a different approach because the T3E run-time system does not allow both MPI and PVM to run concurrently on the same nodes. Therefore, PVM cannot be used on the T3E to manage MPI processes as in the current version of MPI-Connect. On the T3E, a process on a front end must handle all I/O on and off the machine.

Year Three work will include the following:

- performance tuning of communication inside and on/off the machine (e.g., use of multiple paths for I/O on/off the machine to avoid bottlenecks)
- compression and security for communication between machines
- process control on the T3E using the T3E runtime system
- selected MPI-2 I/O features and data management needed for shared virtual files between machines

Deliverables:

- Assist OSU in using MPI-Connect to couple WAM with CH3D in the Year Three CWO Focused Effort
- Finish Cray T3E port of MPI-Connect (May 1998)
- Test and demonstrate interoperation between Cray T3E and other vendor MPIs (June 1998)
- Demonstrate use of MPI-Connect for FMS and other applications (August 1998)
- Contributions to PET bi-weekly and Annual reports (every two weeks according to schedule and March 1999)
- Presentations for PET Mid-Year and Annual Reviews (August 1998, January 1999)
- Tune intra-machine and inter-machine performance (December 1998)
- Workshop on use of MPI-Connect; Test and measure performance on applications (March 1998)
- "Pre-print" report on results of effort (March 1999)

14. Focused Effort Title: High Performance Distributed Object Web based HLA Demonstration

Thematic Area(s): Scalable Computing Migration, HPC Training and DoD User Productivity

PI Name: Dr. David Bernholdt (NPAC-Syracuse)

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Statement of Work: In Year One, Syracuse developed (for ARL MSRC) a Technology Roadmap/Vision for High Performance FMS, based on anticipated Converge of the Web, Distributed Objects, Componentware, HLA, VR and HPDC technologies. In Year Two, Syracuse is accumulating FMS/HLA experience and developing training materials and prototype software components (both for ARL and CEWES MSRCs) that will help to enable the vision outlined in Year One. In Year Three, Syracuse will begin developing metacomputing level HPC FMS demonstrations. In Year Two, Syracuse developed the following software components and interactive training materials in the FMS area:

1) Object Web (Java/CORBA) based RTI (Run-Time Infrastructure) that will facilitate management, monitoring and integration of geographically distributed HLA simulations;
2) Detailed implementation plan for the parallel (Origin2000) port of the Comprehensive Mine Simulator developed by Night Vision Lab at Ft. Belvoir;
3) NPAC installation and hands-on experience with using ModSAF (which provides terrain management for the CMS);
4) Hands-on experience with and interactive training material developed for SPEEDES - an advanced logical time parallel simulation kernel by Caltech-JPL/Metron.
5) Visual Simulation Authoring Tools that will use NPAC WebFlow and DMSO HLA FEDEP standards such as OMT, OML, FOMs, SOMs and DIFs to facilitate high level user friendly development of HLA objects and simulation environments.

In Year Three, Syracuse will develop a HPDC Object Web HLA metacomputing demonstration that will: a) integrate components developed on year 2 and listed above; and b) involve and interconnect FMS users both at ARL and CEWES MSRCs in the cooperative development, testing and simulation fine-tuning activities. The demonstration will use the CMS scenario with one MSRC running the mine field simulation and the other running the tested countermine vehicle. Both simulation components will be packaged as HLA compliant

federates, running on HPC facilities in both centers and communicating across the centers via the Object Web based RTI bus. The implementation of the demonstration described above includes the following steps: a) coarse-grain DIS->HLA conversion of the CMS simulation by wrapping both components as HLA composite federates using Visual Simulation Tools (developed in Year Two); b) installing the Object Web RTI (developed in Year Two) at CEWES MSRC, linking HPC federates at CEWES and ARL MSRCs via the RTI bus, testing and fine-tuning inter-center RTI based communication; c) working with FMS users at both MSRCs to provide the most adequate interactive control, navigation and visualization front-ends. The final demonstration will include support for: a) high end VR controls such as vehicle navigator by MaK Technologies currently used at Ft. Belvoir; and b) Web based lower end but pervasive interface (based on VRML, Java3D or DirectX) that will allow for multi-user access to the simulation from other (Web) sites.

Deliverables:

- Prototype Object Web RTI operational on sequential Java platforms (UNIX workstations, Windows NT PCs) (May 1998)
- HLA version of CMS is operational and tested at NPAC using Object Web RTI (August 1998)
- Contributions to PET bi-weekly and Annual reports (every two weeks according to schedule and March 1999)
- Presentations for PET Mid-Year and Annual Reviews (August 1998, January 1999)
- Both sequential and parallel versions of CMS modules for minefield and tested vehicle installed in respective centers and connected via Object Web RTI. Simple Web browser based control front-end established to both sites/simulation components. Front-end (given by a Java applet with simple 2D navigation tools) allows user to run and monitor distributed CMS from any Web site (December 1998)
- Final Demonstration (March 1999)
- "Pre-print" report on results of effort (March 1999)

15. Focused Effort Title: Web Interfaces for Computational Modules

Thematic Area(s): Scalable Computing Migration, HPC Training and DoD User Productivity

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Statement of Work: This effort has two parts -- a general framework applicable to all applications and a specific application effort applicable to FMS. There is a general need for launching large-grain computations from a simple web interface. Further, in many cases one later wishes to link these as modules in a larger computation where data flows between modules. This can be implemented using conventional Web Server technology (Java applets on clients connected to CGI scripts on servers), but even if this is appropriate today, developments in the object web suggest a powerful model that will fit in with CORBA, IMT/FMS trends to HLA, and increasing use of Java server technology. Syracuse will employ a strategy that allows such coarse-grain objects to be defined in a CORBA fashion on the server side with a Javabean applet front-end. This approach is language independent and will further fit with NPAC's WebFlow technology, which is designed precisely to tackle the dynamic coupling problems identified as critical in the Rice II PET meeting. WebFlow is being linked to the Globus metacomputing framework as part of an NSF sponsored NCSA effort and to CORBA through ARL FMS activity.

Initially, Syracuse will develop a methodology that handles individual modules with a general object framework. This involves:

a) Define a C CORBA wrapper suitable for typical scientific codes. It should have a "run" method, a "display" method (scientists may wish to preserve existing displays) and a set of getparm/setparm methods to find and set parameters. Other input and output methods should also be defined including those needed (eventually) for dataflow. Syracuse assumes C is the most useful language, as codes in FORTRAN can link to CORBA through C. Parallel computations are handled at this stage trivially by using "host-node" model and linking to the host. RIB-like "library" information should also be defined in a natural way.
b) Define a possible domain (FMS, chemistry, environmental quality, etc.) specific Javabean which initially is a container holding one such module at a time and can suitably access methods. It should allow the user to request which module is desired, so it needs to know all available modules. The Javabean and C wrapped module can be

linked by JWORB or general public domain or commercial object brokers supporting C and Java bindings.

With future projects, Syracuse will:

c) Use the JORBed version of WebFlow to implement metacomputing
d) Use the Globus link with WebFlow to allow metacomputing with a visual interface.
e) Use a link to systems such as Nimrod (available in Globus) to control multiple program executions with different datasets
f) Note the natural link to CORBa like HLA, so this is a way of helping FMS users
g) Link to RIB as discussed in NHSE meetings

An FMS application will be the initial target for this project. The application will provide a single, comprehensive access to all application services, including a seamless access to DoD HPC resources. This web-based system will empower local and remote technology use, provide navigation aids for users with varying levels of familiarity with the system, and give access to remote data for browsing and visualization. This new system will be based on industry standard technologies and will reuse legacy as well as commodity software. Syracuse will implement a prototype system that, through a web interface, will allow execution of simulations on a geographically distributed system, including a local host. The front-end of the system will allow the user to specify computational resources to be used, location of the input data sets and the format of the output. The system will upload the specified data to the compute server and launch the application(s) there. The user will control the simulation using the original application's GUI displayed on his/her local display device, and if requested, the output will be feed to a local visualization engine.

Deliverables:

- Initial meeting with FMS group (June 1998)
- Prototype web interface for LMS demonstration (July 1998)
- Report on "lessons learned" from LMS prototype (August 1998)
- Prototype web interface for the Battlefield Assessment and Repair of Roadways demonstration (September 1998)
- Contributions to PET bi-weekly and Annual reports (every two weeks according to schedule and March 1999)
- Presentations for PET Mid-Year and Annual Reviews (August 1998, January 1999)
- Web interfaces ready for demonstration (February 1998)
- Training at CEWES MSRC on Web Interface technology (March 1999)
- "Pre-print" report on results of effort (March 1999)

16. Focused Effort Title: HPC Educational CD-ROM

Thematic Area(s): HPC Training and DoD User Productivity

PI Name: Dr. David Bernholdt (NPAC-Syracuse)

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PI Telephone: (315) 443-3857 **PI Fax:** (315) 443-1973

Statement of Work: NPAC and other PET partners have a sizable volume of educational materials on various areas of HPC which are suitable for asynchronous use, for example by DoD researchers wishing to increase their familiarity with various HPC techniques and tools through self-study. The idea behind this project is to collect such materials into a CD-ROM which can then be distributed to users. This is an on-going effort, guided by an editorial board including Dr. Jack Dongarra, Dr. Geoffrey Fox, Dr. Chuck Koelbel, Dr. Joe Thompson, and Dr. Louis Turcotte. In Year Three, Syracuse will include the following new and revised materials in the CD:

MSU: MPICH, MPIX, MPI++
Rice: Designing and Building Parallel Programs, High Performance Fortran 2
Syracuse: Revised CPS615 (Computational Science for Simulation Applications) course materials
Tennessee: ScaLAPACK, Sparse solvers and preconditioning, Performance evaluation and modeling, Performance optimization, Performance analysis tools

Deliverables:

- Draft CD-ROM for test at JSU (August 1998)
- Master CD-ROM prepared (December 1998)
- Contributions to PET bi-weekly and Annual reports (every two weeks according to schedule and March 1999)
- Presentations for PET Mid-Year and Annual Reviews (August 1998, January 1999)
- CD-ROM produced (1000 copies) (December 1998)

17. Focused Effort Title: Distance Education for Curricula Enhancement

Thematic Area(s): Education, HBCU/MI Interactions

PI Name: Dr. David Bernholdt (NPAC-Syracuse)

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Statement of Work: During Year Two, Syracuse delivered training at CEWES and two full-semester academic courses at Jackson State University. In addition to the academic benefits, this project provided a wealth of practical experience in the design and delivery of educational materials at a distance. In Year Three, Syracuse will deploy these technologies to the DoD community itself in a separate "Distance Training" Focused Effort proposal, but they will also continue and expand work with Jackson State University. Syracuse will expand course offerings to include a graduate level class focused on HPC (Syracuse's CPS615). They will also include other sites by providing technical support to Jackson State University in the remote delivery of courses. After the courses in Year Two, Jackson State is confident that it can deliver using Tango the curricula developed by Syracuse to other HBCU/MI schools. NPAC will provide necessary support for technical and academic content of JSU courses.

Deliverables:

- Deliver CPS615 to JSU (Fall 1998)
- Contributions to PET bi-weekly and Annual reports (every two weeks according to schedule and March 1999)
- Presentations for PET Mid-Year and Annual Reviews (August 1998, January 1999)
- On-going technical support for JSU distance education activities
- "Pre-print" report on results of effort (March 1999)

18. Focused Effort Title: Prototype Distance HPC Training for DoD Users

Thematic Area(s): Training and User Productivity

PI Name: Dr. David Bernholdt (NPAC-Syracuse)

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Statement of Work: The purpose of this effort is to take the lessons learned from prior efforts in Distance Learning and Distance Consulting to develop a prototype capability to provide training classes for MSRC users via the Tango collaborative environment. This effort will identify capabilities not currently available that need to be added; develop approaches to managing training materials and presenting them via Tango; develop procedures to allow MSRC users to participate in Tango-based classes; test and evaluate these approaches and procedures; and conduct one or more "trial" classes with MSRC users demonstrating the prototype capability. For this effort, OSC will provide or develop the training materials for the prototype course and will work with Syracuse to incorporate these materials into a format applicable to Tango. Syracuse will modify the Tango toolset as required to produce the prototype capability in cooperation with OSC.

Deliverables:

- Training course content (April 1998, OSC)
- Training materials in format suitable for Tango (May 1998, OSC)
- Tango training & setup for first training (May 1998, Syracuse)
- Dry run with early recipient sites (June 1998, OSC & Syracuse)
- Distance training delivered to early recipient sites (July 1998, OSC & Syracuse)
- Initial Report (August 1998, OSC & Syracuse)
- Training course content (August 1998, OSC)
- Training materials in format suitable for Tango (September 1998, OSC)
- Tango training & setup for second training (September 1998, Syracuse)
- Contributions to PET bi-weekly and Annual reports (every two weeks according to schedule and March 1999)
- Presentations for PET Mid-Year and Annual Reviews (August 1998, January 1999)
- Dry run with all recipient sites (October 1998, OSC & Syracuse)
- Distance training delivered to all recipient sites (January 1999, OSC & Syracuse)
- "Pre-print" report on results of effort (March 1999)

19. Focused Effort Title: Web-Based Distance Education

Thematic Area(s): HPC Training and DoD User Productivity

PI Names: Dr. Willie G. Brown, Dr. Debasis Mitra, Dr. Qutaibah Malluhi (JSU)

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PI Telephone: (601) 968-2105 **PI Fax:** 601-968-2478

Statement of Work: JSU has established a Web-Based Distance Learning Classroom. In partnership with the NPAC-Syracuse, JSU has offered a Web Programming course, for credit, to undergraduate students during the Fall 1997 and Spring 1998 semesters. This allowed thorough testing and evaluation of the Tango and WebWisdom software environment in a real long distance teaching and learning experiment. The DREN was also used and tested as a delivery infrastructure. In Year Three, JSU will offer a graduate course, for credit, in HPC during the Fall 1998 semester to graduate students. This focused effort will use the same collaboration as in Year 2: NPAC instructors teaching JSU students with JSU faculty and staff assistance. In addition, JSU and Syracuse will recruit at least one other HBCU/MI to participate in the class. This will allow testing of course delivery to multiple sites simultaneously. Also, no later than the Spring 1999 semester, JSU will be the course provider and deliver a course to at least one other HBCU/MI. Finally, in concert with JSU's Scientific Visualization focused effort, JSU will use its facilities to deliver at least one demonstration and at least two workshops to DoD users at the CEWES MSRC.

Deliverables:

- Fall 1998 Graduate Course in HPC, delivered by NPAC to JSU and at least one other HBCU/MI
- Contributions to PET bi-weekly and Annual reports (every two weeks according to schedule and March 1999)
- Presentations for PET Mid-Year and Annual Reviews (August 1998, January 1999)
- Spring 1998 course, delivered by JSU to at least one other HBCU/MI
- At least one Scientific Visualization demonstration, from JSU to the CEWES MSRC
- At least two workshops, from JSU to the CEWES MSRC
- Evaluation, results, lessons learned from all courses presented in final "pre-print" report on effort due on or before 31 Mar 99

20. Focused Effort Title: Scientific Visualization Lab

Thematic Area(s): Scientific Visualization

PI Names: Dr. Willie G. Brown, Dr. Debasis Mitra (JSU)

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Statement of Work: During Year Two, JSU established a Remote SV Laboratory. Mildred Leonard, one of the staff people hired for this lab, spent three months at NCSA, working Dr. Polly Baker and her team. Edgar Powell, the other staff person, spent a great deal of time and effort selecting the proper software and configuring the lab equipment. The goal was to set the foundation for JSU to collaborate with NCSA on SV research and development. In Year Three, JSU will continue collaboration with NCSA, focusing on remote SV. Training will also be provided to JSU faculty, staff, and students in a series of workshops to be conducted by Leonard and Powell. JSU's Web-Based Distance Learning Classroom will allow remote training to other HBCUs/MIs and to CEWES MSRC. During Year Three, JSU will conduct at least one demonstration and at least two workshops to CEWES MSRC personnel. Dr. Debasis Mitra will continue development of an SV course to be delivered via the Web.

Deliverables:

- At least one remote SV demonstration
- At least two SV workshops
- Contributions to PET bi-weekly and Annual reports (every two weeks according to schedule and March 1999)
- Presentations for PET Mid-Year and Annual Reviews (August 1998, January 1999)
- Evaluation, results, lessons learned from SV research and development presented in final “pre-print” report on effort due on or before 31 Mar 99

21. Focused Effort Title: Student Training

Thematic Area(s): HPC Training and DoD User Productivity

PI Names: Drs. O. Olatidoye, S. Sarathy, R. Srikanth, and D. Chen (CAU)

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Statement of Work: There is a need to leverage the ongoing distance learning initiative at CEWES MSRC. CAU will collaborate with Syracuse and Jackson State University to deploy Tango at CAU and evaluate offering the same Tango-based distance education course as JSU for the Fall Semester 1998 using the Virtual Campus infrastructure. In addition, CEWES MSRC needs students for summer projects on location in Vicksburg for 1998. CAU will identify and prepare at least two students for substantial on-site projects at CEWES MSRC during the Summer 1998 timeframe. One of these students may be Mr. Gary Jones, who is assisting CAU on the Residual Capacity of Damaged Structures II effort.

Deliverables:

- CAU submit applicants to participate in the Jackson State Summer Institute in June 1998 (funded by JSU)
- CAU will send at least two students to CEWES MSRC during Summer 1998, one of whom may be the student assistant for the Residual II Focused Effort
- Contributions to PET bi-weekly and Annual reports (every two weeks according to schedule and March 1999)
- Presentations for PET Mid-Year and Annual Reviews (August 1998, January 1999)
- CAU will evaluate offering the same Tango-based distance education course as JSU for the Fall Semester 1998 using the Virtual Campus infrastructure
- Evaluation, results, lessons learned from courses presented and student visits to CEWES in final “pre-print” report on effort due on or before 31 March 1999

22. Focused Effort Title: Residual Capacity of Damaged Structures II

Thematic Area(s): SciVis for Very Large Problems

PI Names: Drs. O. Olatidoye, S. Sarathy and G. Jones (CAU)

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Statement of Work: The focus of this effort is to study the residual life capacity of structures which have been damaged due to explosions or earthquakes. Researchers at CAU will interact and work with the CEWES Structures Laboratory during every phase of this effort. The specific tasks to be accomplished include: (i) a survey and evaluation of various damage rules implemented in CSM CHSSI software; (ii) modeling and simulation of a structure subject to blast loading using this software; (iii) modeling and simulation of a damaged structure due to static/dynamic loading using the software; (iv) visualization of various damage rules using existing MSRC scientific visualization software; and (v) documentation of findings from tasks (i)-(iv). In the first year of this project, CAU performed an assessment of available damage rules in the literature. They also developed a 3-D CAD representation of the DYNA-3D models and developed methods to translate the model data between the different software. They also developed some preliminary concepts to support the visualization of the analysis data within a virtual environment.

In Year Three of the PET program, CAU will further develop and refine techniques to represent the DYNA-3D analysis output in a visualization environment, with particular emphasis on presenting and interpreting damage to the structures. This will mean implementing new damage rules within the software based on the survey of damage assessment methods performed in the first year. This effort will also develop the necessary tools to promote a seamless data exchange between the analysis and modeling components. To effectively portray the damage information, new visual paradigms will be tested within an immersive environment, which will provide greater user interactivity and clarity. An important subtask of this effort (optional) will be to address the seamless integration of existing general purpose unstructured grid generators with this analysis software. This integration will allow analysts to use a consistent modeling interface for geometry definition, specification of analysis attributes, grid generation, analysis execution and the output visualization of the model.

Deliverables:

- Report on the existing damage rules within DYNA-3D (July 1998)

- Complete testbed at ViSiDel. Software to perform conversions between the primary modules (CAD, INGRID, DYNA-3D) for visualization and data exchange installed in testbed (October 1998)
- Report on methods used to visualize damage data in CHSSI SV software (January 1998)
- Contributions to PET bi-weekly and Annual reports (every two weeks according to schedule and March 1999)
- Presentations for PET Mid-Year and Annual Reviews (August 1998, January 1999)
- "Pre-print" report on results of effort (March 1999)

23. Focused Effort Title: Interpretation of Large Data Sets

Thematic Area(s): Management and Interpretation of Large Data Sets

PI Names: Drs. R. Srikanth & R. George (CAU)

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Statement of Work: Advances in data capture and storage have resulted in the generation of vast stores of data in many applications -- scientific and commercial. There is an immediate requirement for a new generation of tools and paradigms to assist humans in the extraction of useful information from this data. This has led to developments in the area of data mining. The fundamental problem addressed by data mining is the interpretation of low "information density" data into forms that have higher information density (i.e., the process of turning data into knowledge). Higher information density models might take various forms-- they might be more compact (for instance, a summary report), be more abstract (a model approximation) or might be more useful (a predictive model). In all these various approaches, there is the application of data mining methods for discovering patterns. In this research, we propose a method of mining databases by combining different paradigms -- genetic algorithms, fuzzy logic and fast clustering algorithms. The objective in this research is to automatically build abstract models that are based on the **interpretation** of underlying large data sets. This research builds upon a previous system, HyGFC (Hybrid Genetic Fuzzy Controller), developed (by one of the PIs) for static generation of knowledge bases from data. Significant extensions to this system that would permit wider applicability in a variety of classification and interpretation tasks are proposed here. This research has important implications for a variety of engineering applications that include failure prediction of structures, decision support, and resource management that require capabilities in automated control, pattern recognition, and machine learning. Fuzzy Logic was initially proposed as a technique to deal with the fundamental impreciseness and uncertainty seen in real-world problems. Two significant benefits result from the use of fuzzy logic for modeling systems: first, the resulting systems are more robust, and second, complex relationships that exist between entities can be modeled more accurately (and easily). These advantages apply to the use of fuzzy logic in data mining, where the data quality cannot be guaranteed. A fundamental step in data mining is the process of data cleaning and data reconciliation. While the application of fuzzy logic to this process does not obviate this stage, it clearly makes the process of mining (i.e., the derivation of abstract models that fit the data) more robust. In this

research, CAU will develop interpretive models based on data mining techniques. CAU will implement the automated generation of such models using Genetic Algorithms. Genetic Algorithms are search procedures based on evolutionary principles. The genetic algorithm will be used to automatically generate such interpretive models rapidly, without recourse to domain information. A feature of data mining problems is that the underlying model is unknown. Impreciseness and uncertainty in the data further complicate this problem. Prediction and classification problems require the extraction of complex relationships that exist between the data components. A fuzzy mode can provide flexibility in representing such relationships and robustness in dealing with noisy data. However, domain information about the problem might be partial or non-existent. Further complicating this process is the high dimensionality of most data mining problems. This necessitates the use of automated techniques of deriving such rule bases. However, the promise of such approaches is that once such interpretive models are extracted and then validated, rapid classification and prediction can be achieved in near real time. The innovative aspect of this effort is that a genetic algorithm is used to integrate all aspects of the interpretive model building -- the definition of both the rule-consequent pairs and tuning of the inferencing process. This provides a solution to applications where the number of variables and the complexity of systems do not permit the acquisition of knowledge from human experts. In such cases automated techniques must be developed for both system identification (i.e., the set of fuzzy rules) and system tuning. In the second part of this research, CAU will investigate the extension of this technique to very large data sets (several hundred megabytes or gigabytes). While this technique is promising for moderate to large data sets, there are obvious problems with much larger data sets. A significant drawback is the time required to validate a model on the data. Alternate techniques that pre-process the data into manageable chunks are required. Traditional clustering is not viable, due to its computational overhead. Efficient search algorithms that fulfill this requirement will be investigated. The approach proposed is generic and problem-independent. That makes it applicable to a variety of domains and problems. This effort will produce an enhancement of the existing HyGFC system developed by the PIs.

Deliverables:

- Pilot analysis of DYNA3D data CAU is using for Residual Capacity of Damaged Structures II effort (August 1998)
- Prototype of enhanced HyGFC in Unix environment (November 1998)
- Addition of clustering algorithms (March 1999)
- Completion of system integration and demonstration of capability using CEWES MSRC output data from DYNA-3D (March 1999)
- Contributions to PET bi-weekly and Annual reports (every two weeks according to schedule and March 1999)

- Presentations for PET Mid-Year and Annual Reviews (August 1998, January 1999)
- "Pre-print" report on results of effort (March 1999)

24. Focused Effort Title: Coupling Sediment, Circulation and Wave Models for Coastal Applications II

Thematic Area(s): Scalable Computing Migration

PI Name: Drs. Keith Bedford and P. Sadayappan (OSU)

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PI Telephone: (614) 292-7338 **PI Fax:** (614) 292-3780

Statement of Work: This effort is a continuation of the Year Two coupling project. The ability to make coupled calculations of combined atmospheric, wave, circulation and sediment transport represents the fullest implementation of HPC modeling activity. Each of these systems has its own characteristic time and length scales and its own associated grid scales and stability characteristics. Often these scales do not overlap, making full coupling difficult. The objectives of this effort are to: (1) complete the process of identifying the most efficient parallel procedures for direct coupling of these models; (2) delineate the time and length scales required for the coupling between the model systems; and (3) determine the frequency of two-way coupling required for model reproduction of field data. This test concentrates on the series of circulation, wave and sediment codes. The codes used for the coupling experiment are WAM, CH3D and SED; the latter being a non-cohesive sediment transport code which predicts multi-class sediment transport and mobile bed dynamics, including sand waves. Much work remains to be done in this area, particularly due to SED not being available in a parallel version and the presence of the mobile bed component of the model, which places considerable emphasis on wave-current-bed interaction formulation. The three parallel codes -- WAM, CH3D, and SED -- will be applied to the OSU Lake Michigan test basin for run for idealized and hindcast observed meteorological conditions. As it was in Year Two, the degree of coupling frequency required for realistic simulation will be a critical variable to determine.

Deliverables:

- Verify WAM and CH3D parallelizations (June 1998)
- Implement WAM/CH3D coupling in parallel on T3E (September 1998)
- Complete parallelization of SED and implementation in CH3D (December 1998)
- Contributions to PET bi-weekly and Annual reports (every two weeks according to schedule and March 1999)
- Presentations for PET Mid-Year and Annual Reviews (August 1998, January 1999)
- "Pre-print" report on results of effort (March 1999)

25. Focused Effort Title: Parallelization of SED (Joint with MSU)

Thematic Area(s): Scalable Computing Migration

PI Name: Drs. Keith Bedford and P. Sadayappan (OSU)

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PI Telephone: (614) 292-7338 **PI Fax:** (614) 292-3780

Statement of Work: The accumulation, movement and destruction of cohesive sediment is a potentially critical component in modeling estuarine, lake and coastal environments. The nature of such deposits are that their composition and distribution can alter rapidly in response to the prevailing marine, meteorological and inflow/outflow conditions. At present, there is no parallel cohesive sediment code available at CEWES MSRC. This project will address this issue by parallelizing the SED model.

The CFD program at MSU will take the lead in performing the parallelization of SED. OSU will deploy the code in the Lake Michigan testbed and test its performance relative to the sequential version. OSU will first deploy the sequential SED using a 4km Lake Michigan grid and idealized hindcast test cases. The code will then be parallelized with accuracy and scalability evaluated using the same testbed.

Deliverables:

- Deployment of sequential SED on Lake Michigan (November 1998)
- Deployment of parallel SED on Lake Michigan (March 1999)
- Contributions to PET bi-weekly and Annual reports (every two weeks according to schedule and March 1999)
- Presentations for PET Mid-Year and Annual Reviews (August 1998, January 1999)
- "Pre-print" report on results of effort (March 1999)

26. Focused Effort Title: Prototype Distance HPC Training for DoD Users

Thematic Area(s): Training and User Productivity

PI Name: Dr. Charlie Bender and Ms. Leslie Southern

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Statement of Work: The purpose of this effort is to take the lessons learned from prior efforts in Distance Learning and Distance Consulting to develop a prototype capability to provide training classes for MSRC users via the Tango collaborative environment. This effort will identify capabilities not currently available that need to be added; develop approaches to managing training materials and presenting them via Tango; develop procedures to allow MSRC users to participate in Tango-based classes; test and evaluate these approaches and procedures; and conduct one or more "trial" classes with MSRC users demonstrating the prototype capability. For this effort, OSC will provide the training materials for two prototype courses and will work with Syracuse to incorporate these materials into a format applicable to Tango. Syracuse will modify the Tango toolset as required to produce the prototype capability in cooperation with OSC. The courses will consist of two 2-day curricula from one of the following options:

- Parallel Programming on the CEWES MSRC Cray T3E
- Parallel Programming on the CEWES MSRC SGI O2000
- Parallel Performance Optimization
- Fortran 90

Deliverables (OSC):

- Training course content, first course (April 1998)
- Training materials in format suitable for Tango, first course (May 1998)
- Dry-run with recipient sites, first course (June 1998)
- Distance training delivered, first course (July 1998)
- Initial Report (August 1998)
- Training course content, second course (August 1998)
- Contributions to PET bi-weekly and Annual reports (every two weeks according to schedule and March 1999)
- Presentations for PET Mid-Year and Annual Reviews (August 1998, January 1999)
- Training materials in format suitable for Tango, second course (September 1998)
- Dry-run with recipient sites, second course (October 1998)
- Distance training delivered, second course (December 1998)
- "Pre-print" report on results of effort (March 1999)

27. Focused Effort Title: A Coupled Hydrodynamic-Water Quality Model Based on ADCIRC3D and CE-QUAL-ICM

Thematic Area(s): Scalable Computing Migration

PI Names: Drs. Mary Wheeler and Clint Dawson (TICAM-Texas)

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Statement of Work: TICAM will work with DoD personnel in developing a prototype hydrodynamic flow/water quality model in two dimensions. This prototype will be based on two DoD codes, ADCIRC and CE-QUAL-ICM. The latter code was recently parallelized by University of Texas and DoD personnel, and the parallel version is currently being validated on the Chesapeake Bay data set. TICAM is also currently developing a parallel version of ADCIRC3D, based on earlier work performed on a two-dimensional version of ADCIRC. TICAM will have a prototype parallel version of the code by the end of Contract Year Two, but validation of the code will continue into Contract Year Three. The prototype coupling code will require the following:

1) A two-dimensional hydrodynamic projection code must be implemented which takes the velocity output from ADCIRC and creates a “locally conservative" velocity field (such a velocity field is necessary for the water quality model). A projection algorithm has already been derived and analyzed, but only a prototype code testing the algorithm has been studied. TICAM will first implement a code which computes a locally conservative velocity on a CE-QUAL-ICM grid.

2) TICAM will further investigate, with DoD researchers, algorithms suitable for water quality modeling on unstructured prismatic elements in two and three dimensions.

Deliverables:

- Validated version of parallel ADCIRC3D (June 1998)
- Parallel hydrodynamic projection code (November 1998)
- Contributions to PET bi-weekly and Annual reports (every two weeks according to schedule and March 1999)
- Presentations for PET Mid-Year and Annual Reviews (August 1998, January 1999)
- User's manual and training (March 1999)
- "Pre-print" report on results of effort (March 1999)

28. Focused Effort Title: An Example of Launching a Parallel Simulation Under the Groundwater Modeling System (GMS)

Thematic Area(s): HPC Training and DoD User Productivity

PI Names: Dr. Mary Wheeler (TICAM-Texas)

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PI Telephone: (512) 475-8625 **PI Fax:** (512) 471-8694

Statement of Work: PARSIM (Parallel Aquifer and Reservoir Simulator) is a 3D flow and transport simulator for modeling contamination and remediation of soils and aquifers. It was developed at the University of Texas at Austin. The code uses sophisticated numerical methods for solving the flow and transport equations and includes very general reaction kinetics, including geochemical and biogeochemical processes. The code is fully parallelized using domain decomposition and MPI and is operational on the IBM SP and Cray T3E platforms. PARSIM is currently being incorporated into GMS, and programming tools required to "launch" PARSIM on any of the parallel hosts at CEWES MSRC are being developed. As a first prototype of launching, Texas has created tools appropriate for executing PARSIM on a single computing environment. For this effort, Texas will further investigate more complex programming tools such as GLOBUS, which provides the tools needed to execute in a metacomputing environment.

Deliverables:

- Launching prototype on a single parallel platform (May 1998)
- User's manual completed and training session (July 1998)
- Contributions to PET bi-weekly and Annual reports (every two weeks according to schedule and March 1999)
- Presentations for PET Mid-Year and Annual Reviews (August 1998, January 1999)
- Report on metacomputing environments (January 1999)
- "Pre-print" report on results of effort (March 1999)

29. Focused Effort Title: Adaptive Mesh Technology Applied to Damaged Structures

Thematic Area(s): Scalable Computing Migration

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Statement of Work: The purpose of this project is to introduce and promote unstructured grid approaches and adaptive grid technology to Computational Structural Mechanics (CSM) codes. The work will be developed in two phases.

During Phase 1 (June – October 1998), TICAM will:
1) examine the framework and existing software for CSM applications to complex problems such as those involving simulation of hypervelocity impact using CTH and similar software such as EPIC;
2) investigate the limitations of adaptive approaches to these applications and determine appropriate strategies to improve the analysis capability;
3) begin work on *a posteriori* feature and error indicators for guiding mesh refinement; and
4) communicate with researchers at Sandia National Laboratories Albuquerque (SNLA) regarding related unstructured grid and adaptive grid research activities.

Provided the results of Phase 1 indicate the feasibility of proceeding further, Phase 2 will be implemented. During Phase 2 (November 1998 – March 1999), the TICAM researchers will:
1) investigate and delineate strategies for applying adaptive mesh techniques to these CSM applications (both short term and longer-term approaches);
2) carry out research on appropriate unstructured grid and adaptive grid approaches;
3) ascertain, through analysis and pilot studies, the improvements in computational efficiency, accuracy and reliability (for a specified accuracy level) of CSM applications using these adaptive schemes;
4) continue work on *a posteriori* error indicators;
5) begin work to implement basic indicators in a software module; and
6) initiate work on an Applications Program Interface (API) between the adaptive mesh software and the CSM applications.

This work will involve interaction with David Littlefield at the Army Institute for Advanced Technology (IAT), with DoD users, and with other analysts involved in related ASCI work on unstructured grids and adaptive grids.

TICAM will proactively communicate their findings among DoD users, the CEWES MSRC, IAT and SNLA. A short course on unstructured grids, adaptive grids and *a posteriori* error analysis will be given by TICAM during the period of performance.

Part of the development work will address issues of compatibility of existing data structures in current analysis codes for unstructured grids, refining and re-meshing. TICAM will investigate strategies for developing an API to meet the Adaptive Mesh Refinement (AMR) objective. A software module will be designed and tested during Phase 2 that includes representative feature and error indicators and that can be expanded subsequently.

Deliverables:

- Contributions to PET bi-weekly and Annual reports (every two weeks according to schedule and March 1999)
- Presentations for PET Mid-Year and Annual Reviews (August 1998, January 1999)
- Contributions to the PET CSM web page on adaptive algorithms, test problems, error analysis, etc.

Phase 1:

- Lectures at DoD meeting (Rice University) on Topics in Finite Element Methodology. (This will include material on adaptive grids and error indicators as well as other topics of interest to the PET program, CSM and other applications.) (June 1998)
- Briefing to CEWES MSRC on initial studies and interactions with collaborators (August 1998)
- Research report on analysis of limitations and efficiency of adaptive strategies, data structures and implementation issues, approach for API design (October 1998)

Phase 2:

- "Pre-print" report on results of effort to cover work on *a posteriori* error indicators, data structures, API interface, indicator software module and related work carried out under the project (March 1999)

30. Focused Effort Title: Benchmarking HPC Systems II

Thematic Area(s): HPC Performance Metrics/Tools

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Statement of Work: Recently, several new HPC architectures and software systems to program these have been introduced. In these, many architectural features are hidden from the application developers, while visible features may not always be exploited by the end users to compare the performance of these machines in a meaningful way. Indeed, such comparisons are difficult to understand and involve complex interplay between the architecture, the application domain, the expertise of the user, the amount of effort that the user is willing to spend to optimize performance, portability as well as software legacy issues.

The goal of this project is to define a set of useful parameters to evaluate the performance of state-of-the-art HPC platforms for stressing DoD applications. Of particular interest is the new generation of shared memory systems (bus based as well as coherent cache based systems), whose performance modeling and tuning is challenging compared with message passing systems. USC will take a two-stage approach by first defining a set of basic parameters to understand architectural features from an application mapping perspective and then using these to map a large scale DoD application code to be specified by the sponsor. This effort will continue the previous one begun in the latter part of Year Two, producing an interim report during the first half of Year Three, then a final report.

Deliverables:

- Interim research report detailing the performance parameters of shared memory machines and comparison of parallelization of a DoD application with current implementation of the same application on a message passing machine (August 1998)
- Contributions to PET bi-weekly and Annual reports (every two weeks according to schedule and March 1999)
- Presentations for PET Mid-Year and Annual Reviews (August 1998, January 1999)
- "Pre-print" report on final results of effort (March 1999)

Appendix C: Points of Contact for CEWES MSRC PET Program

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